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Anisotropic mesh adaptation in Firedrake with PETSc DMPlex

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Abstract

Despite decades of research in this area, mesh adaptation capabilities are still rarely found in numerical simulation software. We postulate that the primary reason for this is lack of usability. Integrating mesh adaptation into existing software is difficult as non-trivial operators, such as error metrics and interpolation operators, are required, and integrating available adaptive remeshers is not straightforward. Our approach presented here is to first integrate Pragmatic, an anisotropic mesh adaptation library, into DMPlex, a PETSc object that manages unstructured meshes and their interactions with PETSc's solvers and I/O routines. As PETSc is already widely used, this will make anisotropic mesh adaptation available to a much larger community. As a demonstration of this we describe the integration of anisotropic mesh adaptation into Firedrake, an automated Finite Element based system for the portable solution of partial differential equations which already uses PETSc solvers and I/O via DMPlex. We present a proof of concept of this integration with a three-dimensional advection test case.
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1. Introduction

As the size of the numerical simulations required by both the industry and research sectors continues to grow, anisotropic mesh adaptation is an efficient means to reduce the CPU time of the computations while improving their accuracy [1,4,10]. However, it is still not widely adopted in the solvers community due to the difficulty of integrating it to partial differential equation solver frameworks. Various adaptive mesh processes can be found in the literature, but they all remain complex to set up. They require several complex steps: computation of an element size and orientation map, generation of a mesh with respect to this map and solution transfers, which are often implemented in different codes that have to be combined. Adaptation for transient problems is even more complex, as these steps often have to be repeated many times.

In PETSc, the widely used scientific library providing data structures and routines for the parallel solution of partial differential problems [2], the mesh management library DMPlex [7] aims at making application code developers' lives easier by providing them with a wide set of tools to manipulate unstructured meshes, thus avoiding the need to write

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such specialized routines. Integrating Pragmatic [6], an anisotropic mesh adaptation library, into DMPlex is a first step towards making mesh adaptation available to a larger community, as it offers the possibility to easily generate and use adapted meshes within application codes which make use of PETSc. As an example, Firedrake [11], a system for the portable automated solution of partial differential equation based problems, is one such code considered here. Providing routines for mesh adaptation in this framework would make it even more accessible.

The purpose of this research note is to present the integration of Pragmatic to Firedrake via DMPlex and the implementation of a full mesh adaptation algorithm with Firedrake, which are the first steps towards fully automated mesh adaptation. We first present the three codes involved, and show how they are integrated. The chosen adaptation strategy is then described, and demonstrated using a 3D advection problem.

2. Presentation of the codes involved

Firedrake. Firedrake is a code for the automated solution of Finite Element problems [11]. It is based on a strict division into different abstraction layers, each layer being concerned with a specific task: definition of the problem, local discretization defining the data structures and kernels to compute the solution, and the parallel execution of these kernels. Different kinds of optimization can be applied at each level, from caching of mathematical forms to compiler-level optimization in the kernels, including data sorting. The definition of the problem is done using a domain-specific language (DSL) for the specification of partial differential equations in variational form. This allows the user to define very simply their problem, with a language close to the underlying mathematical description. A wide range of finite element types and degrees are supported. Efficient parallel execution of the numerical kernels on unstructured mesh data is performed by a framework where parallel loops are expressed at a high level, and which uses its own representation of the data as sets and maps. Finally, the resulting linear or non-linear systems are solved via the PETSc library, which is also used for the handling of unstructured meshes via DMPlex.

PETSc and DMPlex. DMPlex is the PETSc object which manages unstructured meshes using a Hasse diagram representation and directed acyclic graph data structure [7]. The library has a wide variety of tools for mesh traversal and manipulation, including submesh extraction, partitioning and distribution, I/O, and parallel load balancing. DMPlex uses a uniform topological interface, meaning that vertices, edges, facets and cells are treated equally as points of the graph representation (see Fig. 1). This allows algorithms which operate independent of dimension, cell type, cell mixture, or partitioning. A key point is that topological operations can be directly translated to graph operations, which is ideal for optimization and parallelization. DMPlex also provides an abstraction for associating function spaces with pieces of the mesh, allowing the user to construct approximations like finite elements and finite volumes which are made of small spaces pieced together. Firedrake uses DMPlex for mesh representation, to organize traversals in the global approximation space, and to interface with advanced solvers, such as unstructured multigrid and block preconditioners. The way DMPlex enables efficient handling of unstructured meshes is detailed in [8].
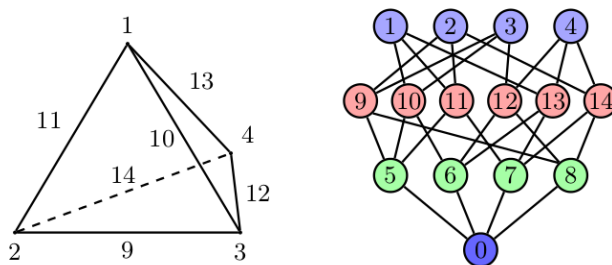

Fig. 1: Example of DMPlex representation for a single tetrahedron.

Pragmatic. Pragmatic is a 2D and 3D anisotropic local remesher, that generates a unit mesh with respect to a prescribed metric field [6]. The adapted mesh is obtained from the input mesh through a series of local mesh manipulations: iterative applications of refinement, coarsening and edge/face swapping optimise the resolution and the quality

of the mesh, and quality-constrained Laplacian smoothing fine-tunes the mesh quality. An interface between DMPlex and Pragmatic was developed in this work. This enables PETSc users to adapt an unstructured mesh to a specified metric field with only one call. The DMPlex object is converted into Pragmatic data structures, and a new DMPlex is created from its output. The advantage of this approach is that it allows application codes to interface with mesh adaptation through an I/O like interface, thereby making the integration of mesh adaptation much less intrusive in the application code.

3. Transient adaptation algorithm

To demonstrate the solution we consider the global fixed-point adaptation algorithm described in [3] , based on:

- the subdivision of the simulation interval into n_{adap} sub-intervals: $[0, T] = [0 = t^1, t^2] \cup \ldots \cup [t^i, t^{i+1}] \cup \ldots \cup [t^{n_{adap}}, t^{n_{adap}+1} = T]$, on each of which we consider a unique adapted mesh,
- an iterative process to converge the mesh/solution couple and to address prediction of the solution issues.

An overview of the algorithm is presented in Algorithm 1. On each sub-interval $[t^i, t^{i+1}]$, we consider a mean Hessian of the solution u : $\mathbf{H}_u^i(\mathbf{x}) = \int_{t^i}^{t^{i+1}} |H_u(\mathbf{x}, t)| \, dt$. The d-dimensional adapted mesh on sub-interval i is generated from the following metric, which has been proven to be optimal for the control of the L^p interpolation error:

$$\mathcal{M}_{L^p}^i(\mathbf{x}) = \mathcal{N}_{st}^{\frac{2}{d}} \left(\sum_{j=1}^{n_{adap}} \mathcal{K}^j \left(\int_{t^j}^{t^{j+1}} \tau(t)^{-1} dt \right)^{\frac{2p}{2p+d}} \right)^{-\frac{2}{d}} \left(\int_{t^i}^{t^{i+1}} \tau(t)^{-1} dt \right)^{-\frac{2}{2p+d}} (\det \mathbf{H}_u^i(\mathbf{x}))^{-\frac{1}{2p+d}} \mathbf{H}_u^i(\mathbf{x}) , \tag{1}$$

where $\mathcal{K}^i = \int_{\Omega} \left(\det \mathbf{H}_u^i(\mathbf{x}) \right)^{\frac{p}{2p+3}} d\mathbf{x}$, $\tau(t)$ is a function of time specifying the time-step and $\mathcal{N}_{st}$ is the target space-time complexity (the number of space-time vertices). $\mathcal{N}_{st}^{\frac{2}{d}} \left(\sum_{j=1}^{n_{adap}} \mathcal{K}^j \left(\int_{t^j}^{t^{j+1}} \tau(t)^{-1} dt \right)^{\frac{2p}{2p+d}} \right)^{-\frac{2}{d}}$ is a global normalization term that enables an optimal distribution of the number of vertices on the sub-intervals. It requires that the problem is solved on the whole simulation interval before the metrics for each sub-interval can be computed. The steps of Algorithm 1 are detailed in the following Section.

Algorithm 1 Mesh Adaptation Algorithm

Given: Initial mesh and solution, target space-time complexity
For $j = 1, n_{ptfx}$ *// Fixed-point loop to converge the mesh/solution couple problem*
  1. For $i = 1, n_{adap}$ *// Adaptive loop to advance the solution in time on time frame* $[0, T]$
     (a) Interpolate the solution from the previous sub-interval;
     (b) Compute the solution on sub-interval;
     (c) Compute sub-interval averaged Hessian from Hessian samples;
    EndFor
  2. Compute global normalization term and all sub-interval metrics;
  3. Generate all sub-interval adapted meshes;
EndFor

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4. Implementation of the algorithm

Metric computation. The metrics from Equation (1) are based on the mean Hessian of the solution. Instead of computing the Hessian for each solver time-step, we only average samples, typically 20 per sub-interval. The Hessian, H, is computed using a classic Galerkin method. We desire H such that: $H = D^2 u$, which can be written in weak form, for a test function τ in the appropriate function space Σ:

$$\int_{\Omega} \tau : (\sigma + D^2 u) \, dx - \int_{\partial \Omega} \tau : (\mathbf{n} \otimes \nabla u) \, ds = 0, \quad \forall \tau \in \Sigma . \tag{2}$$

This can be easily written in the high-level language of Firedrake, and then is automatically solved. The samples are then averaged on the fly, and the resulting mean Hessian for the sub-interval is stored. At the end of the simulation-interval, the normalization term can be computed and the final metrics for each sub-interval obtained.

Generation of adapted meshes. The meshes are generated by Pragmatic, whose integration with Firedrake via DM-Plex is explained in Section 2. For each sub-interval, the DMPlex object corresponding to the current mesh is sent to PETSc together with the metric field, and PETSc returns a DMPlex object corresponding to the new adapted mesh.

Solution transfer. Between two sub-intervals, the solution has to be transferred from one mesh to the following. For now, we use the point evaluation mechanism from Firedrake: given any point in the domain, it provides the value of a given function at this point. Since we are considering Lagrange P^1 finite elements, a linear interpolation is performed, in the computational space.

5. Numerical example

We consider the 3D advection of a bubble, first introduced in [9]. This case is usually used as a demonstrator for interface-tracking methods. Here, we show that mesh adaptation allows us to limit considerably the spurious diffusion of the solution.

We consider the scalar advection equation for a quantity u in a 3D domain Ω:

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \tag{3}$$

where $\mathbf{v}$ is a velocity field defined on Ω. The computational domain is a $[0,1] \times [0,1] \times [0,1]$ cube. At $t = 0$, $u = 0$ everywhere except in a ball of radius 0.35 centered in $(0.35, 0.35, 0.35)$, which models the bubble and where $u = 1$. The following velocity field is considered, so the bubble quickly becomes distorted:

$$\mathbf{v}(x, y, z, t) = \begin{cases} 2\sin^2(\pi x)\sin(2\pi y)\sin(2\pi z)\cos(2\pi t/T) \\ -\sin(2\pi x)\sin^2(\pi y)\sin(2\pi z)\cos(2\pi t/T) \\ -\sin(2\pi x)\sin(2\pi y)\sin^2(\pi z)\cos(2\pi t/T) \end{cases}, \tag{4}$$

where T is the period. Here $T = 6$, and the simulation is run until $t = 1.5$.

Equations (3) and (4) are solved using a Lagrange P^1 Finite Element method. A SUPG stabilization method is used, with a Crank-Nicolson scheme employed for advancing in time. This is easily achieved thanks to Firedrake: one just has to write the variational formulation in the high-level language, and the corresponding low-level solver is automatically generated.

The global fixed-point algorithm from Section 3 was used, with $n_{adap} = 25$ sub-intervals and 3 global iterations. This way, only 25 adapted meshes are used for the whole simulation interval, and only 50 adapted meshes are generated. Snapshots of the meshes and solutions at the last fixed-point iteration are shown in figure 2. The meshes have an average size of $406, 571$ vertices, ranging from $273, 061$ to $557, 586$. One can clearly see the adapted band-shaped regions, as well as the accuracy of the solution, that exhibits little numerical diffusion.

The whole simulation was run serially, as the code is not yet fully parallelized. However, it was run in 32 hours on one core, which shows the efficiency of the approach and the potential power when run with more cores.

6. Conclusion

We have shown how a transient mesh adaption algorithm was successfully implemented using Firedrake, PETSc DMPlex and Pragmatic. The long-term goal is to fully integrate mesh adaptivity within Firedrake's core, so that it can be used by application developers with only a few lines of code. The main ongoing improvement tracks include the parallelization of the whole process and the extension of this work to more complex finite element spaces. Most tasks are already automatically parallelized in Firedrake, what remains is the parallelization of the interface between DMPlex and Pragmatic, for which parallel I/O support will have to be added in DMPlex. Extending adaptivity to higher degree or other kinds of Finite Elements notably requires improving the solution transfer procedure, and we aim at using the Supermesh library [5] to this end.
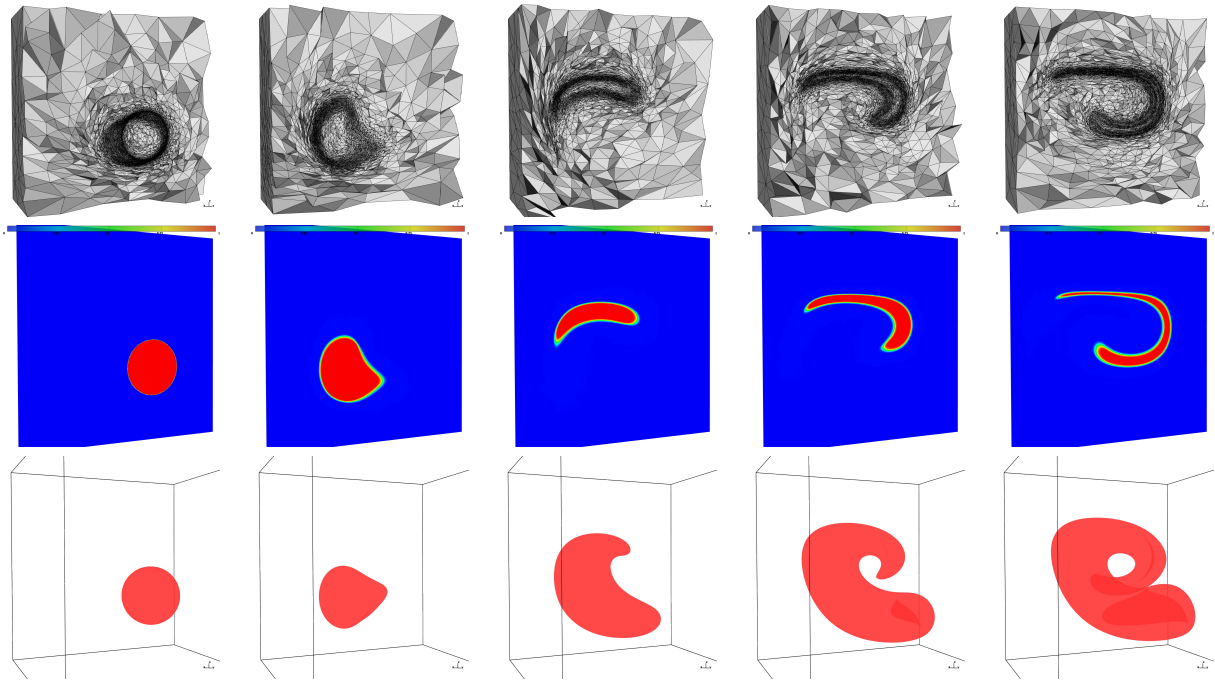
Fig. 2: Cuts in the mesh (top) and solution (middle) at dimensionless times $t = 0, 0.24, 0.54, 0.84$ and 1.5. Isosurfaces of the solution (bottom) at the same times are also given.

Acknowledgements

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